

WHAT IS CLAIMED IS:

1. A method for assaying multi-component mixtures comprising:

a. introducing light from a wide-band source of optical radiation and dividing the light into spectral components, and/or extracting the assigned sections of monochromatic light with a spectral width of Δ_i from the light in the selected range of wave-lengths λ_i while ensuring the possibility of changing the spectral position of these sections with the assigned pitch $\Delta\lambda_i \geq \Delta_i$;

b. Focusing the extracted monochromatic light onto a probing beam having a specified geometric shape, and directing the light onto a sample under analysis;

c. Irradiating a sample of a known mixture K and a sample of an unknown mixture U , by turns, with monochromatic light at the assigned wave-lengths $\lambda_1, \lambda_2, \dots \lambda_m$ from the selected spectral range λ_i ;

d. Collecting and directing light falling onto the sample, passing through the sample, or reflected by the sample, and the luminescent light to independent photo-detector devices;

e. Measuring the intensity values of the light gathered on the photo detector for each of the extracted wave-lengths $\lambda_1, \lambda_2, \dots \lambda_m$ of the selected spectral range

λ_i , such that, the probing light I_0 , the light passing through a sample or reflected by a sample I_T , and the luminescence light of a sample I_L , including steps of decomposition of the luminescent light into a variety of spectral sections, and/or sequential extraction of the specified sections of wave-lengths of $\lambda_1, \lambda_2, \dots \lambda_n$ with a width of Δ_j , with the assigned pitch of $\Delta\lambda_j \geq \Delta_j$, where each section corresponds with the predetermined characteristic wave-length of the light in the selected spectral range λ_j , which is gathered and registered by a photo-detector is measured;

f. Defining the relative intensity of the gathered light passing through a sample, or reflected by a sample, at each of extracted wave-lengths λ_m , and the luminescent light for each of the extracted wave-lengths λ_m, λ_n for a known mixture and unknown mixture, in accordance with the following expressions:

$$T^K(\lambda_m) = \frac{I_T^K(\lambda_m)}{I_0^K(\lambda_m)}; \quad T^U(\lambda_m) = \frac{I_T^U(\lambda_m)}{I_0^U(\lambda_m)};$$

$$L^K(\lambda_m, \lambda_n) = \frac{I_L^K(\lambda_m, \lambda_n)}{I_0^K(\lambda_m)}; \quad L^U(\lambda_m, \lambda_n) = \frac{I_L^U(\lambda_m, \lambda_n)}{I_0^U(\lambda_m)}, \text{ where}$$

$I_T^K(\lambda_m), I_T^U(\lambda_m)$ - intensity values of passing or reflected light for samples of a known K mixture and an unknown U mixture measured within the specified sections $\lambda_1, \lambda_2, \dots$

λ_m of the extracted range of wave-lengths of incident radiation λ_i ;

$I_L^K(\lambda_m, \lambda_n), I_L^U(\lambda_m, \lambda_n)$ - intensity values of the luminescent irradiated by a sample of a known K mixture and a sample of an unknown U mixture within the specified sections $\lambda_1, \lambda_2, \dots \lambda_n$ of the extracted range of wave-lengths λ_j with light excitation within the specified sections $\lambda_1, \lambda_2, \dots \lambda_m$ of the extracted range of wave-lengths λ_i ;

$I_0^K(\lambda_m), I_0^U(\lambda_m)$ - intensity values of incident probing radiation falling on the appropriate samples at the time of performing measurements;

g. Comparing the corresponding relative intensity values of the light passing through a sample, or reflected by a sample, on each of extracted wave-lengths λ_m , and the luminescent light for each of the extracted wave-lengths λ_m, λ_n for a known mixture and an unknown mixture, and defining the compliance between the unknown mixture and the known mixture by the following expression:

$$A = \frac{1}{2} \times \left(\frac{1}{m} \times \sum_{m=1}^m \frac{T^U(\lambda_m)}{T^K(\lambda_m)} + \frac{1}{m \times n} \times \sum_{m=1}^m \sum_{n=1}^n \frac{L^U(\lambda_m, \lambda_n)}{L^K(\lambda_m, \lambda_n)} \right) = 1 \pm \delta, \text{ where}$$

$T^K(\lambda_m), T^U(\lambda_m)$ - intensity values of passing or reflected light for samples of a known K mixture and unknown U mixture, normalized for the intensity of incident radiation

falling on a sample at the corresponding wave-length;

$L^K(\lambda_m, \lambda_n), L^U(\lambda_m, \lambda_n)$ - intensity values of the luminescent light irradiated by a sample of a known K mixture and unknown U mixture within the specified sections $\lambda_1, \lambda_2, \dots \lambda_n$ of the extracted range of wave-lengths λ_j with light excitation within the specified sections $\lambda_1, \lambda_2, \dots \lambda_m$ of the extracted range of wave-lengths λ_i , normalized for intensity of incident radiation falling on a sample at the corresponding wavelength;

m, n - a number of extracted sections with the wave-lengths under compared within the selected spectral ranges λ_i and λ_j , accordingly;

δ - a value of allowable deflections of the compared values for the unknown mixture being identified from the corresponding values for the similar values of a standard sample of a known mixture;

h. Defining the presence or absence of foreign impurities in the mixture by the following expressions:

$$C_r(\lambda_i) = \frac{T^U(\lambda_{m+1})}{T^K(\lambda_{m+1})} - \frac{T^U(\lambda_m)}{T^K(\lambda_m)}; \quad C_L(\lambda_i, \lambda_j) = \frac{L^U(\lambda_{m+1}, \lambda_{n+1})}{L^K(\lambda_{m+1}, \lambda_{n+1})} - \frac{L^U(\lambda_m, \lambda_n)}{L^K(\lambda_m, \lambda_n)},$$

at the same time, if $C_r(\lambda_i) = C_L(\lambda_i, \lambda_j) = 0 \pm \delta$, foreign impurities in the sample being identified are absent, and the conclusion about the presence of unwanted contaminations

in the mixture under study may be drawn when there are sections $C_T(\lambda_i) > 0 \pm \delta$, and/or $C_L(\lambda_i, \lambda_j) \neq 0 \pm \delta$ in the difference spectra.

2. A method for analyzing a sample comprising multi-component mixture comprising:

- a. Obtaining an electronic absorption-luminescent signature of the multicomponent mixture;
- b. Comparing the electronic absorption-luminescent signatures of the sample with the electronic absorption-luminescent signature of a known mixture;
- c. Preparing calibration samples which represent a specially made-up mixture or multi-component solution of a strictly identical constant compound, the absorption or reflectance spectra, and luminescence spectra of which solution (mixture) overlap with the corresponding spectra of a known mixture within the selected analytical spectral ranges λ_i and λ_j , i.e. have nonzero intensity in the specified ranges;
- d. Placing a standard sample of a known K mixture and a calibration Q sample into an analytical device;
- e. Measuring and transforming measured values for intensity of the light passing through or reflected by standard and calibration samples, and their luminescent light, in accordance with steps a-f of claim 1, while

taking into account the step of replacing an unknown U sample with the calibration Q sample;

f. Creating an electronic absorption-luminescent signature ALS_K of a standard sample as follows:

$$ALS_K = \|K_E\| = \begin{vmatrix} \left(\frac{T_1^K}{T_1^Q} \right) \left(\frac{L_{1,1}^K}{L_{1,1}^Q} \right) \dots \left(\frac{L_{1,n}^K}{L_{1,n}^Q} \right) \\ \dots \\ \left(\frac{T_m^K}{T_m^Q} \right) \left(\frac{L_{m,1}^K}{L_{m,1}^Q} \right) \dots \left(\frac{L_{m,n}^K}{L_{m,n}^Q} \right) \end{vmatrix}, \text{ where:}$$

$T^K(\lambda_m), T^Q(\lambda_m)$ - intensity values of passing or reflected light for a sample of a known K mixture and a sample of a calibration Q mixture, normalized for intensity of incident radiation falling on a sample at the corresponding wave-length;

$L^K(\lambda_m, \lambda_n), L^Q(\lambda_m, \lambda_n)$ - intensity values of the luminescent light irradiated by a sample of a known K mixture and a calibration Q mixture within the specified sections $\lambda_1, \lambda_2, \dots \lambda_n$ of the extracted range of wave-lengths λ_j with light excitation within the specified sections $\lambda_1, \lambda_2, \dots \lambda_m$ of the extracted range of wave-lengths λ_i , normalized for intensity of incident radiation falling on a sample at the corresponding wave-length;

g. Entering the electronic signature of a standard sample ALS_K into a computer database, and/or saving the electronic signature of the standard sample on an inter-

mediate medium;

h. Repeating step (e) with a sample of an unknown mixture, including the step of replacing a standard sample K with a calibration sample Q , which is strictly identical with the calibration sample used when measuring a standard sample, and creating an electronic signature ALS_U of a sample being identified:

$$ALS_U = \|U_E\| = \left\| \begin{pmatrix} \frac{T_1^U}{T_1^Q} & \left(\frac{L_{1,1}^U}{L_{1,1}^Q} \right) & \left(\frac{L_{1,n}^U}{L_{1,n}^Q} \right) \\ \vdots & \vdots & \vdots \\ \frac{T_m^U}{T_m^Q} & \left(\frac{L_{m,1}^U}{L_{m,1}^Q} \right) & \left(\frac{L_{m,n}^U}{L_{m,n}^Q} \right) \end{pmatrix} \right\|;$$

i. Comparing electronic signatures of an unknown mixture $ALS_U = \|U_E\|$ being tested with similar data for a standard sample of a known mixture $ALS_K = \|K_E\|$ by the following expression:

$$\|A_{ALS}\| = \frac{\|U_E\|}{\|K_E\|},$$

such that, a conclusion on the identity of the unknown mixture and the certain mixture may be drawn when all cells of the matrix $\|A_{ALS}\|$ contain only unit elements (i.e.

$$a_i = a_{i,j} = 1 \pm \delta;$$

j. Defining the presence or absence of unwanted con-

taminations for the mixture under study by the following expression:

$$\|C_{ALS}\| = \frac{\|U_E\| - \|K_E\|}{\|K_E\|},$$

at the same time, a determining the presence of unwanted contaminations in the mixture $\|C_{ALS}\|$ when in the matrix there are nonzero elements $|c_i, c_{i,j}| > |\pm\delta|$, the values of which exceed the value of allowable deflections of the values being compared for the unknown mixture being identified, from the corresponding values for the similar values of a standard sample of a known mixture;

3. The method according to claim 1 further comprising measuring intensity values of Raman scattering of the identified sample and a standard sample including the following steps:

a. irradiating the samples an unknown and a known mixture, by turns, with a monochromatic line of a narrow-band (lined) source of light at one or several selected fixed frequencies ν_r ;

b. Gathering the light of Raman scattering onto a photo-detector device;

c. Measuring the intensity of the light on each of the extracted frequencies $\nu_1, \nu_2, \dots, \nu_p$ of the selected spectral range, gathered onto a photo-detector, namely:

the exciting light falling on a sample I_{ex} , and the light of Raman scattering of a sample I_R , including steps of decomposition of the light of Raman scattering into a variety of spectral sections, and/or sequential extraction of the specified frequency sections $\nu_1, \nu_2, \dots, \nu_p$ with a width of Δ_r , with assigned pitch $\Delta\nu_r \geq \Delta_r$, where each section corresponds to the predetermined characteristic frequency of the light in the selected spectral range ν_r , which is gathered and registered by a photo-detector;

d. Defining the relative intensity of the gathered light of Raman scattering at each of the extracted frequencies $\nu_1, \nu_2, \dots, \nu_p$ for a known and unknown mixtures in accordance with the following expressions:

$$R^K(\nu_{ex}, \nu_p) = \frac{I_R^K(\nu_{ex}, \nu_p)}{I_{ex}^K}; \quad R^U(\nu_{ex}, \nu_p) = \frac{I_R^U(\nu_{ex}, \nu_p)}{I_{ex}^U};$$

where:

$I_R^K(\nu_{ex}, \nu_p), I_R^U(\nu_{ex}, \nu_p)$ - intensity values of Raman scattering irradiated by a sample of a known K mixture and a sample of an unknown U mixture within the specified sections $\nu_1, \nu_2, \dots, \nu_p$ of the extracted frequency range ν_r with light excitation at one of the selected frequencies ν_{ex} ;

I_{ex}^K, I_{ex}^U - intensity values of the exciting light falling on corresponding samples at the time of performing

measurements;

e. Comparing data for the mixture being tested with similar data for a standard sample of a known mixture by the following expression:

$$A = \frac{1}{2} \times \left(\frac{R^U(\nu_{ex}, \nu_p)}{R^K(\nu_{ex}, \nu_p)} \right) \times \left(\frac{1}{m} \times \sum_{m=1}^m \frac{T^U(\lambda_m)}{T^K(\lambda_m)} + \frac{1}{m \times n} \times \sum_{m=1}^m \sum_{n=1}^n \frac{L^U(\lambda_m, \lambda_n)}{L^K(\lambda_m, \lambda_n)} \right),$$

the unknown mixture and the known mixture are identical when $A = 1 \pm \delta$.

4. The method according to claim 2 comprising comparing electronic signatures containing spectral profiles of absorption, luminescence and Raman scattering intensities for the mixture (RALS_U) and a standard sample (RALS_K), which electronic signatures are formed by the method of claim 3, wherein the Raman matrixes are normalized in the following way:

a. Preparing a calibration sample Q_R , which calibration sample represents a specially made-up mixture or a multi-component solution of a strictly identical constant compound, the luminescence spectrum of which overlaps with the Raman spectrum of the known mixture within the selected analytical spectral ranges;

b. Measuring the intensity of Raman scattering, converting the results as in steps d-h of claim 2, and forming the electronic Raman signatures of a standard sample

and the unknown mixture being identified in accordance with the following expressions:

$$\|K_R\| = \left\| \begin{pmatrix} R_{1,1}^K \\ \vdots \\ R_{q,1}^K \end{pmatrix} \dots \begin{pmatrix} R_{1,p}^K \\ \vdots \\ R_{q,p}^K \end{pmatrix} \right\| \quad \text{and} \quad \|U_R\| = \left\| \begin{pmatrix} R_{1,1}^U \\ \vdots \\ R_{q,1}^U \end{pmatrix} \dots \begin{pmatrix} R_{1,p}^U \\ \vdots \\ R_{q,p}^U \end{pmatrix} \right\|, \quad \text{where}$$

$R_{q,p}^K, R_{q,p}^U$ - intensity values of Raman scattering light, normalized for intensity of the exciting light I_{ex} , for samples of the known K mixture and the unknown U mixture, measured at the frequencies I_p with light excitation at the frequency I_q ;

$L_{q,p}^{Q_R}$ - the luminescence intensity for a calibration sample Q_R , normalized for the intensity of the exciting light I_{ex} ;

c. Comparing the electronic signatures of the unknown mixture $\|U_E\|$ being tested with similar data for a standard sample of a known mixture $\|K_E\|$, including the step of comparing electronic Raman matrixes (RAL_{U,K}), by the following expression:

$$\|A_{RAL}\| = \left(\frac{\|U_R\|}{\|K_R\|} \right) \times \left(\frac{\|U_E\|}{\|K_E\|} \right),$$

where the identity of samples is defined by the following attribute: $\|A_{RAL}\| = 1 \pm \delta$.

5. The method according to claim 1 wherein samples of the mixture being identified and the standard mixture are dissolved in appropriate solvents.

6. The method according to claim 1 wherein the mixture being analyzed is water.